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Mapping future soil carbon change and its uncertainty in croplands using simple surrogates of a complex farming system model

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ABSTRACT

Soil organic carbon (SOC) in agricultural soils is vital for soil fertility for sustainable agricultural production and climate change resilience. Process-based farming system models are widely used to predict SOC dynamics in agricultural soils, but their application at regional scales is largely limited by computational requirements, data availability, and uncertainties in model predictions. Here we present an approach of combining a farming system model and a simplified surrogate model that emulates and mimics the behaviour of complex process-based models to predict SOC change (ΔSOC) and its uncertainty in Australian dryland cropping regions under anticipated climate change. We first calibrated and validated the farming system model APSIM for simulating ΔSOC (0–30 cm soil) using data from 90 farming-system trials at 28 sites across the study regions. Next we conducted a comprehensive simulation across the region using the validated APSIM model to predict ΔSOC over the period 2009–2070. Then simple surrogate models were developed based on the APSIM outputs. The surrogate models were able to explain > 96% of the variation in APSIM-predicted ΔSOC. Last the surrogate models were applied across the regions at the resolution of 1 km. In our simulations, Australian dryland cropping soils under farmers' common management practices and future climate conditions were a net carbon source (0.66 Mg C ha^{-1} with the 95% confidence interval ranging from −5.79 to 8.38 Mg C ha^{-1}) during the 62-year period. Across the regions, simulated ΔSOC exhibited great spatial variability ranging from −108.8 to 9.89 Mg C ha^{-1} at the resolution of 1 km, showing significant ($P < 0.05$) negative correlation with baseline SOC level, temperature and rainfall, and positive correlation with pasture frequency (the duration of pasture in the rotation divided by the whole duration of the rotation) and nitrogen application rate. The uncertainty in ΔSOC and the underlying drivers were also assessed. This study presented a novel approach to efficiently predict future SOC dynamics and their uncertainty at fine resolutions, facilitating the development of site-specific management strategies for soil carbon sequestration.

1. Introduction

Conservation of soil organic carbon (SOC) in agricultural soils is vital for sustainable agricultural production and mitigating climate change (Bradford et al., 2016; Kahiluoto et al., 2014; Lal, 2004). SOC usually declines after land use change to cropping (Sanderman et al., 2017) until a lower steady state is reached. Synthesising global data sets, Guo and Gifford (2002) estimated the decline in SOC to be in the order of 42–59% when natural systems were converted to cropland. Similarly, Luo et al. (2010) estimated that Australian cropping soils

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have lost 50–60% of the initial SOC stocks in top 30 cm that were present before land clearing. However, detailed SOC dynamics in different regions depend on agricultural management practices, and vary with soil and climate conditions. Conservation agriculture practices such as stubble retention, no-tillage, organic amendments, avoidance of long fallow periods, and increased crop rotation complexity (e.g., the introduction of legumes and cover crops) have been recommended to reduce SOC declines or to enhance carbon sequestration (Gan et al., 2014; Luo et al., 2010; Smith, 2016; West and Post, 2002). More recently, the international initiative "4 per 1000" aims at a yearly 4‰ increase of SOC in global agricultural soils to ensure food security and mitigate climate change (Minasny et al., 2017). However, this ambitious target has been challenged by the soil carbon research community because of uncertainties surrounding carbon predictions across spatio-temporal scales and resource requirements such as financial support for farmers to change agricultural practices to sequester carbon (Baveye et al., 2018; Vandenbygaart, 2018; White et al., 2018). It is vital to elucidate SOC dynamics across space and time under various cropping systems and management practices, particularly under climate change, to enable a realistic assessment of the likelihood of being able to improve SOC stocks (or minimise losses).

Numerous experimental studies have been conducted to assess the response of SOC to various agricultural management practices, and it has been widely accepted that practices that increase organic matter input into the soil can reduce SOC losses or sequester more carbon (Freibauer et al., 2004; Luo et al., 2010; West and Post, 2002). In addition, the quality of organic matter inputs, local climate and soil conditions may regulate the trend of SOC change after adopting those practices due to their effects on SOC losses via microbial decomposition (Kong et al., 2005; Luo et al., 2017a). Nevertheless, manipulated field experiments can only consider limited variations in crop rotations and associated management practices such as residue removal and fertilizer application, making it difficult to extrapolate experimental findings to field conditions across a number of regions with different soils and climate. In Australia's grain-cropping regions, for example, farmers' choices of crop rotations and management practices depend on local climate, soil and market conditions, resulting in diverse cropping systems. To account for > 99% of the cropped area in Australia, it has been suggested that 22 crops should be included in the national carbon accounting system (Unkovich et al., 2009). Considering the many possible crop sequences and their varying impact on SOC, it is impractical, if not impossible, to use field experiments to investigate the SOC dynamics influenced by this large number of crop species grown under different rotations and management across regions that contain a range of soils and climates. A modelling approach is best suited for such purposes.

Agricultural system models with well-tested crop and soil modules enable the investigation of the impact of alternative management scenarios, climate variability and future climate change on the productivity of agricultural systems and SOC dynamics. A large number of studies have used such strengths of agricultural system models to simulate SOC dynamics under various conditions in terms of soil, climate and agricultural management (Kucharik et al., 2001; Liu et al., 2009; Luo et al., 2011; Qiu et al., 2009). In general, modelling results suggest that carbon inputs are the predominant factor influencing the SOC balance in agricultural soils (Wang et al., 2016; Zhao et al., 2013). However, most modelling studies have focused on the verification of models for simulating SOC dynamics under specific cropping systems (including rotations) at the plot scale. When applying the model to larger spatial scales, model predictions may suffer from large uncertainties induced by model structure, parameter equifinality, and limited data availability for model initialization/parameterization (Luo et al., 2015; Ogle et al., 2010b; Saby et al., 2008). Thus, extending plot-scale modelling to analyse SOC dynamics over space and time relies not only on the availability of information required for the modelling, but also on the capability of the models to simulate the growth of various crops and their interaction with management practices, and SOC decomposition processes across environments.

In this study, we combined the Agricultural Production Systems sIMulator (APSIM) (Holzworth et al., 2014) and surrogate modelling to predict future SOC dynamics over 62 years in Australian dryland cropping regions. The APSIM model allows flexible specification of management options such as crop and rotation type, tillage, residue management, and fertilizer application, and has the capacity to simulate the interaction of crop growth and soil processes with soil, climate and management practices. In the present study, the APSIM model was first constrained for simulating SOC dynamics using observational data sets collected from the major dryland cropping regions across Australia. Then the constrained model was applied to simulate SOC dynamics during the period 2009–2070 under farmers' current common management practices (i.e., business-as-usual) at 1869 sites across the study region. The uncertainty in model predictions was also assessed. Based on the APSIM simulation results, we developed surrogate models of the APSIM model to predict the spatial pattern of SOC change across large regions at fine resolution. Surrogate modelling derives simple relationships driven by easily obtainable information to mimic results of complex process-based models (Luo et al., 2013; Marie and Simioni, 2014). Surrogate models have the advantage of requiring much less information than complex models like APSIM, facilitating the application of the model across large spatial scales in terms of both lower computational cost and data requirements. Specifically, the objectives of the study were to: 1) predict SOC dynamics from 2009 to 2070 under various management practices under future climate change conditions using the constrained APSIM model; 2) quantify whether and how future SOC changes correlate to local soil and climate conditions and management practices; and 3) present and assess a surrogate modelling approach to represent the complex APSIM model, and 4) implement the surrogate model to assess the spatial pattern of SOC change in Australia's cereal-growing regions at 1 km resolution.

2. Materials and methods

2.1. Study region and representative cropping systems

This study focuses on Australian rainfed cropping areas identified from the map of Land Use of Australia 2010–11 at the resolution of 1 × 1 km (Fig. 1). This cropping area includes a total of ~260,000 grid cells (1 × 1 km), accounts for ~3% of the total area of Australia, and is spread across 23 different Agro-Ecological Regions (AERs) (Williams et al., 2002) (Fig. 1), and cover a wide range of climatic and soil conditions. Specifically, the annual average temperature across the region ranges from 6.5 to 28.2 °C, precipitation from 124.7 to 4291.0 mm, and SOC in the top 0.3 m soil from 11.8 to 264.1 Mg C ha^{-1}. For each AER with cropping, a crop rotation (Table S1) was derived based on data from Australian Bureau of Statistics for the period from 2010 to 11 to 2014–15. Along with the crop rotations, the relevant fertilizer use and crop residue management were calculated using the Yield and Nitrogen Calculator (Baldock, 2012) and from the Australian crop and pasture management database (Unkovich & Baldock 2017, unpublished data), respectively. In brief, these crop rotations and the relevant management represent current common agricultural management in each AER. The details on compiling this information are provided in Supplementary Material and Methods S1.

2.2. Soil and climate data

Soil data (0–2 m) was obtained from the database of the Soil and Landscape Grid of Australia (SLGA, http://www.clw.csiro.au/aclep/soilandlandscapegrid/). The SLGA is derived based on digital soil mapping methods and integrates historical soil data, new measurements with spectroscopic sensors, and novel spatial modelling (Grundy et al., 2015). The SLGA provides detailed soil attributes at the

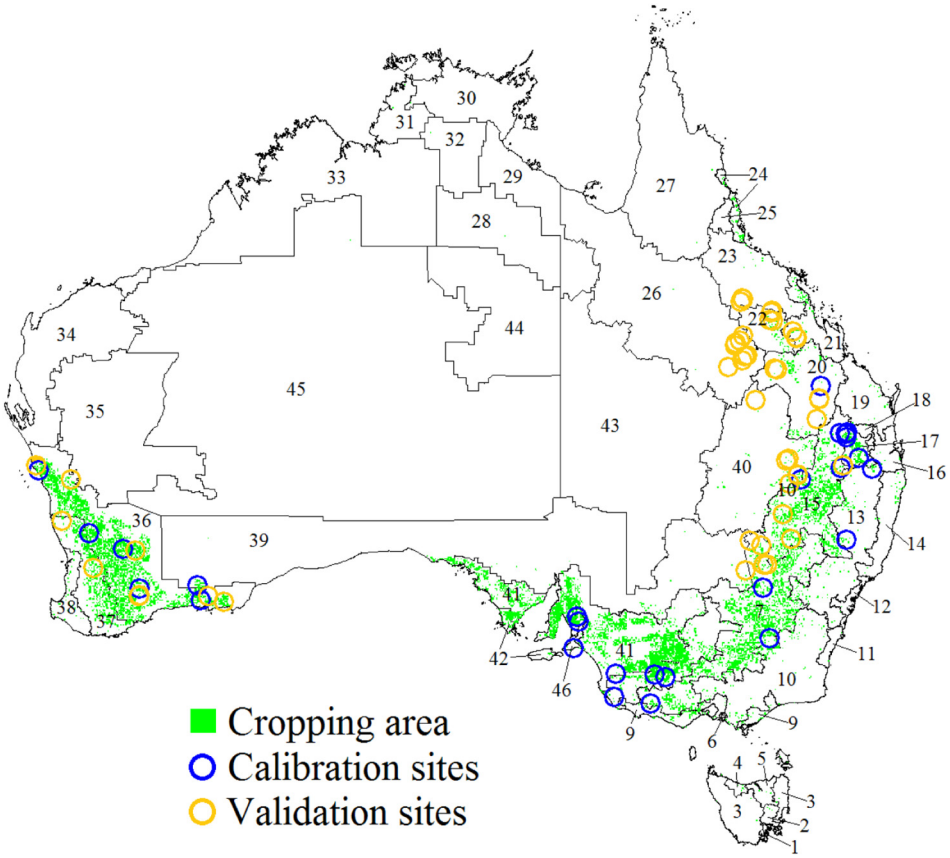

Fig. 1. The study region. Green pixels show rainfed cropping areas in Australia. Blue and orange circles show the sites where data were used to calibrate and validate the APSIM model, respectively. The boundary with the number code show the 46 agro-ecological regions (AER). See Williams et al. (2002) for the name of each AER. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

resolution of 3 arcsecond (~90 × 90 m) across Australia. In this study, we extracted the soil parameters in the 0–2 m soil profile including soil layers (e.g., 0–0.1 m, 0.1–0.3 m, the detailed layer depth is location-dependent) with soil bulk density, SOC and nutrient contents, hydraulic properties (saturation water content (SAT), drained upper limit (DUL), 15 bar lower limit (LL15)), and pH for each soil layer. These layered parameters were used to initialize the APSIM model for SOC simulations (see below). More details about the soil data are provided in Supplementary Materials and Methods S2.

Projected climate data from five Global Circulation Models (GCMs), obtained from PCMDI (the Program for Climate Model Diagnosis and Intercomparison) and WGCM (the WCRP's Working Group on Coupled Modelling), were downscaled to a total of 8023 climate sites using NWAI-WG, a weather generator-based statical downscaling model developed at NSW DPI's Wagga Wagga Agricultural Institute (Liu and Zuo, 2012). In our study, we used RCP 4.5, a moderate emissions scenario (Van Vuuren et al., 2011) for modelling SOC changes over a period of 62 years from 2009 to 2070. As CO_2 concentration is required for the APSIM model to simulate the response of crop growth to elevated atmospheric CO_2 concentration, we also estimated the CO_2 concentration for each year using an empirical equation proposed by Liu et al. (2017). The details of the downscaling approach are given in Supplementary Materials and Methods S3.

2.3. The APSIM model

We used the Agricultural Production Systems sIMulator version 7.5 (APSIM) to simulate SOC dynamics. The APSIM model provides accurate predictions of crop production as influenced by climate, crop cultivars, soil properties and management assumptions for sowing, irrigation, fertilization, and tillage, and has the capability of simulating > 30 crops (Holzworth et al., 2014; O'Leary et al., 2016). The model simulates crop growth and soil processes on a daily time-step in response to climate (e.g., temperature, rainfall, radiation, and atmospheric CO_2 concentration), soil water availability, and soil N and phosphorus status. The performance of the APSIM model in simulating crop growth (Asseng et al., 1998; Meinke et al., 1997; Wang et al., 2003) and SOC dynamics (Huth et al., 2010; Luo et al., 2011; Luo et al., 2015; Probert et al., 2005) has been widely and explicitly tested and verified under different cropping and management systems at many locations and over long time periods for Australian conditions. This history of model verification gives a sound basis for the use of the model in this study. In this study, we further constrained the APSIM model for simulating SOC dynamics using data sets collected across the study regions (see the next section below).

In APSIM, the SoilN module simulates SOC dynamics – coupling with modules for soil water (SoilWat), surface organic matter (SurfaceOM), and plant growth. The SoilN module divides total SOC into four conceptual pools: fresh organic matter (FOM), microbial biomass (BIOM), humic organic matter (HUM), and inert organic matter (IOM). Except for IOM which is not decomposable, the decomposition of the other three pools is treated as a first-order decay process with the decay rate modified by soil moisture and temperature, and soil N availability, leading to the release of CO_2 to the atmosphere and the transfer of the remaining organic matter to other pools. The relative fraction of CO_2 emissions and the remaining C is defined in terms of C use efficiency (which is the amount of C used for microbial growth relative to total C consumed). The flow of nitrogen depends on the C:N ratio of the receiving SOC pool. Decomposition of surface residue is simulated by the SurfaceOM module, taking into account the degree of contact of residue with soil and the C:N ratio of the residue to modify the maximum potential decomposition rate specified according to residue type. A fraction of decomposed residues contributes to soil BIOM and HUM pools, and the remainder leaves the system as CO_2. Nitrogen can be mineralized or immobilized to or from the mineral N pools depending on the C:N ratio of the residues and receiving SOC pools. When

surface residues are incorporated into the soil via tillage, they are treated as FOM input for the SoilN module.

2.4. Model calibration and validation

Before conducting our simulations, we first calibrated the APSIM model for simulating SOC dynamics using observational data from 90 agricultural trials at 28 sites across the study region (Fig. 1). The data set includes detailed records on crop sequence, and agricultural management practices such as residue management (removal or retention) and fertilizer application for each year. These data were used to specify crop management in the APSIM model. Most of the soil properties required to initialize soil conditions had been measured at the start of the experiments, including total nitrogen content, bulk density, clay content and pH. For other variables (soil hydraulic variables) that were unavailable but required for model initialization, we adopted the values from the nearest SLGA (the soil database) point. SOC stock in each experiment was determined for representative 0–0.3 m soil samples at least at the beginning and end of the experiments. All the data sets used in this study were from the calibration and enhanced paired sites reported by Skjemstad and Spouncer (2003) and are available at: http://www.fullcam.com/FullCAMServer/Help/reps/ (Report No. 36).

The SOC stock data were used to calibrate the performance of the APSIM model in simulating SOC dynamics. The aim of the calibration is to ensure that the model can reasonably capture the observed SOC dynamics across the region using a common set of model parameters. The calibration focused on three most important soil-related parameters/inputs influencing SOC dynamics, the coupled nitrogen dynamics and crop growth (Luo et al., 2015): the fraction of inert organic carbon (*finert*), the decomposition rate of humic organic carbon (k_{hum}), and the microbial carbon use efficiency (*CUE*, which is defined as the efficiency with which microbes use substrate for biosynthesis). We used a Bayesian optimization approach to optimize the three parameters in order to obtain the best performance of the APSIM model in simulating observed SOC stocks. First, for each of the three parameters we assumed an empirical uniform distribution bounded with a range (0–1 for *finert*, 0.0015–0.000015 day^{-1} for k_{hum}, and 0.2–0.8 for *CUE*) that is biologically and physically possible. Then, the model was optimized using a differential evolution algorithm for global optimization (Mullen et al., 2009) to best match the observed SOC data sets. The mean residual sum of squares was minimized to target the best agreement between model predictions and observations. Finally, we obtained 100 ensembles of optimized parameters (i.e., k_{hum}, *finert*, and *CUE*,), representing the joint posterior distribution of the three parameters enabling the estimation of the uncertainty induced by parameter equifinality (that is, a model using different ensembles of parameters can equally well simulate observations) (Luo et al., 2015; Tang and Zhuang, 2008).

Although the APSIM model can well simulate crop growth (Fig. S1) using the optimized posterior distributions of the three parameters, we did not use the simulated aboveground C input during the calibration. Rather, during the calibration the recorded aboveground C input (as crop residue) was manually incorporated into the model at the time of crop harvesting, whilst the simulated crop residue was removed. This manipulation eliminated the effect of an imperfect match of modelled with observed crop residue (Fig. S1) on SOC dynamics and therefore on the estimation of model parameters.

After calibrating the model, we used an independent data set to validate APSIM-simulated SOC dynamics at another 46 sites (Fig. 1) using the calibrated model parameters. This validation data set was also reported by Skjemstad and Spouncer (2003), their “new paired sites”, and are also available at: http://www.fullcam.com/FullCAMServer/Help/reps/ (Report No. 36). All model set up, initialization and running for model validation followed the same procedure as that for model calibration.

2.5. APSIM simulations

After obtaining the 100 ensembles of optimized parameters that can equally-well simulate observed SOC across the study region, the APSIM model was run continuously from 2009 to 2070 using each parameter ensemble under the five climate projections (Table S2) at 1869 points randomly selected across the study region (Supplementary Materials and Methods). As such, there are a total of 500 simulations for each point, resulting in ~60 million simulation years. To complete these simulations, 31.5 h were required by parallel computing using 1000 modern computer cores (CSIRO Bragg Cluster). Due to this significant computational cost, we did not conduct a spatially-explicit simulation (~180 days required if running the model at each of the ~260,000 grid cells). Rather, we developed a surrogate model to estimate APSIM-predicted SOC dynamics (see the surrogate model development section below). Except for the three optimized parameters (i.e., k_{hum}, *CUE* and *finert*), all other initial soil information required by the APSIM model was derived from the SLGA database as described above.

Depending on the AER to which the simulated point belongs, the corresponding crop rotation (Table S1) in that AER was repeated over the 62-year simulation. Sowing time was determined by soil moisture. The starting and ending sowing date varied based on the sowing window for each crop by the Agriculture department of each state in Australia. Cultivars were assigned according to sowing date—the earlier the sowing date is, the later the maturity type of the crop cultivar selected. Three cultivars for each crop representing early, middle and later maturity cultivars were selected from the listed default cultivars in the parameter files released with the crop modules in the APSIM model. Perennial pasture was simplified due to the lack of information on species grown at the experimental sites and simulated as a lucerne cultivar *Trifecta* – the most common sown pasture species in Australia. Fate of crop residues (stem plus leaf) after harvest was based on the database on residue management (see supplementary Materials and Methods). The perennial lucerne was sown after harvest of annual crops and ploughed into the soil before sowing the next crop. Harvest to the height of 10 cm was assumed whenever lucerne reached the flowering stage to mimic grazing by livestock. We acknowledge that mis-specified sowing rules and cultivars may lead to some uncertainties in biomass production and thereby C inputs to the soil. However, this would not be a significant issue as the dominant factors controlling biomass production are soil nutrient availability and climate conditions. All other management actions relating to residue management and fertilizer application were specified using the inventory data described in supplementary materials and methods. As these simulations were based on management information from statistical, survey and/or inventory databases reflecting current common agricultural management practices, these simulations can be referred to as the business-as-usual simulation.

2.6. Assessing the uncertainty in predicted SOC change

Soil organic carbon stocks in the top 30 cm soil were outputted for each year during the 62-year simulation. For each point, the absolute SOC change (ΔSOC) from 2009 to 2070 was calculated for each of the 500 simulations (i.e., 500 ΔSOC for each point were obtained), which were used to estimate the average and 95% confidence interval (CI, i.e., the 2.5% and 97.5% quantiles of the 500 estimates) of ΔSOC at each point. The 95% CI of predicted ΔSOC represents the uncertainties induced by model parameter equifinality and uncertainties in climate projections at each point. We estimated the relative contribution of parameter equifinality and climate projection to total uncertainties at each point using the approach in Ogle et al. (2010a, 2010b). First, total variance of the 500 estimates (V_T) was partitioned into variance among five climate projections (V_C) and variance among 100 parameter ensembles within climate projections (V_P), i.e., $V_T = V_C + V_P$. Then, the relative contributions of parameter equifinality and climate projection were calculated as $V_P/V_T \times 100\%$ and $V_C/V_T \times 100\%$, respectively.

We also estimated the national average Δ*SOC* using a bootstrapping approach. The mean of Δ*SOC* across the 1869 points was estimated as:

$$\theta_i = \frac{\sum_{j,k} \theta_{i,j,k}}{n},\ n = 1869 \quad (1)$$

where $\theta_{i,j,k}$ is the *i*th bootstrapping prediction of Δ*SOC* for the *j*th point (which is a random draw from the 1869 points with replacement) and the *k*th simulation in that point (which is a random draw from the 500 simulations considering uncertainties in model parameters and climate projection). We conducted 5000 bootstraps to ensure the convergence of the bootstrapping samples. Based on the 5000 estimates, the average and 95% CI were calculated, representing the national average Δ*SOC* and its uncertainty respectively. To compare the differences in Δ*SOC* under different climate projections, the bootstrapped average and 95% CI of Δ*SOC* for each climate projection were also calculated. If the 95% CI of Δ*SOC* under a climate projection does not overlap with the 95% CI under another climate projection, it indicates that Δ*SOC* is significantly different between the two climate projections. For each AER, we only reported the average and standard deviation of all simulated Δ*SOC* because some AERs have limited simulation points, making it impossible to do bootstrapping.

2.7. Surrogate model development to capture APSIM predictions

In order to facilitate spatially-explicit predictions of Δ*SOC* across the study region, we developed a surrogate model to mimic the APSIM-predicted Δ*SOC*. The surrogate model has the advantage of not requiring detailed information to initialize the process-based APSIM model and saves computing time. In addition, the simulated Δ*SOC* at each simulation point across the diverse soil, climate and management conditions provides an opportunity to address whether and how the simulated Δ*SOC* correlate with climate, soil conditions, and cropping systems. This information is critical to understand SOC dynamics across space and time. For the development of the surrogate model, we focused on the simulated average Δ*SOC* at each point, i.e., the response variable of the surrogate model. We hypothesized that Δ*SOC* associates with local soil and climate conditions. We focused on one soil property [i.e., initial SOC stock at the start of the simulation (C_0)], and two climate variables [i.e., mean annual precipitation (MAP) and temperature (MAT)]. For MAP and MAT, we used the value during the period 1976–2005 (to make it consistent with data obtained from the Bureau of Meteorology of Australia, see the surrogate model implementation section below) rather than during the simulation period 2009–2070. Although this may sacrifice the model performance to some extent, an apparent advantage of using historical MAP and MAT is that they are easily available and based on real climate records, eliminating the effect of uncertainty in climate projections. Additionally, it facilitates the application of the surrogate model across the region. At the same time, we assumed that the detailed relationships between Δ*SOC* and the three soil and climate variables vary among the 23 AERs (i.e., 23 crop systems), and the characteristics of the crop rotation and management practices in each AER affect Δ*SOC*.

We calculated five variables to indicate the characteristics of cropping systems: the relative frequency of pasture seasons in the crop rotation (*fP*, which was calculated as the seasons of pasture in the rotation divided by the whole duration of the rotation), the relative frequency of grain legume crops (*fL*), the relative frequency of fallow periods (*fF*), the average nitrogen fertilizer application rate (*rN*, which was calculated as the total fertilizer input amount divided by the duration of the rotation), and the removal fraction of crop residues (*rR*, i.e., the fraction of crop resides that were not returned to the soil). When calculating *fP*, *fL* and *fF*, a year was divided into two seasons (i.e., winter and summer cropping seasons). So, for example, for a 5-year crop rotation system, there are 10 seasons. If there are two seasons of legumes, five seasons of fallow and three seasons of pasture, then *fL* = 0.2, *fF* = 0.5 and *fP* = 0.3. Table S1 shows the detailed crop rotations, which were used to calculate *fL*, *fF*, and *fP* for each AER.

A linear mixed-effects model (Gelman & Hill, 2006) (hereafter called surrogate model) was fitted with random effects for C_0, *MAT* and *MAP* and fixed effects for *fP*, *fL*, *fF*, *rN* and *rR*. The surrogate model can be generally written as:

$$y_{i,j} \sim \alpha_j + \beta_j \cdot X_{i,j} + \gamma \cdot Z_j + \varepsilon, \quad (2)$$

where $y_{i,j}$ is the APSIM-predicted Δ*SOC* in the j^{th} AER/cropping system, α_j the model intercept, β_j the coefficient vector of random effects which varies with AER/cropping system, $X_{i,j}$ the predictor vector (i.e., C_0, *MAT* and *MAP*) of random effects, γ the coefficient vector of fixed effects which is constant for all AERs/cropping systems, Z_j the predictor vector (i.e., *fP*, *fL*, *fF*, *rN* and *rR*) of fixed effects, and ε the error. In essence, there is a separate regression model for each AER with its coefficients of random effects estimated by the weighted average of pooled (which do not consider groups, i.e. a traditional fixed-effect model) and un-pooled (which consider each group separately) estimates, i.e. partial pooling. As a result, we obtained 23 group-level coefficients for each group-level predictor which vary among the 23 AERs (i.e., 23 cropping systems). The surrogate model was fitted using the *lmer* function in the *arm* package in R 3.3.2 (R Core Team, 2016). A repeated 10-fold cross-validation (i.e., the 10-fold cross-validation was repeated 10 times in this study) was applied using the *cvFit* function in the *cvTools* package in R. The final model was selected with minimum prediction error [i.e., the root mean squared error (RMSE)] using the *cvSelect* function in the *cvTools* package. When performing these statistics, all independent variables were standardized using *z-scores*. In addition to the surrogate model to predict average Δ*SOC*, two other surrogate models were also developed to predict the lower and upper limits of the 95% CI of Δ*SOC* using the same approach and predictors.

2.8. Implementation of the surrogate model across Australian rainfed cropping regions

After obtaining the surrogates to mimic APSIM-predicted average Δ*SOC* and its uncertainty (i.e., the lower and upper limits of the 95% CI), we applied these surrogates across the whole Australian rainfed cropping regions at the resolution of 1 km (Fig. 1). For each 1 km grid cell, initial SOC stock C_0 was extracted from the SLGA database. As the SLGA database is at the resolution of ~90 m, we calculated C_0 as the average of SOC in all 90 m cells located within in the targeted 1 km grid cell for Δ*SOC* estimation. MAT and MAP data during the period 1976–2005 were obtained from the Bureau of Meteorology of Australia at the resolution of 5 km (http://www.bom.gov.au/climate/averages/maps.shtml), and the closest MAT and MAP to the simulated 1 km grid cell was used. Depending on which AER the simulated grid cell belongs to, the five predictors representing cropping systems in that AER were used. Finally, we obtained three maps at the resolution of 1 km showing the average Δ*SOC* and its upper and lower limits of 95% CI predicted by the surrogates of the APSIM model. Since the surrogates were able to explain > 97% of APSIM predictions (see details in Results section), we did not estimate the uncertainty induced by the surrogate models.

3. Results

The APSIM model adequately simulated the observed SOC stocks in the top 30 cm soil layer (Fig. 2). Pooling together all data of the 90 experiments, the calibrated APSIM model could explain 83% ($P < 0.001$) of the variance in observed SOC stocks (Fig. 2a). Using the 100 different ensembles of the three parameters (Fig. 2b), model performance was nearly identical evidenced by the very small error bars in Fig. 2a. The posterior range of the three model parameters (k_{hum}, *finert*, and *CUE*) spanned a wide range (Fig. 2b). This occurred because k_{hum}, *finert*, and *CUE* were closely correlated with each other (Fig. 2b). This

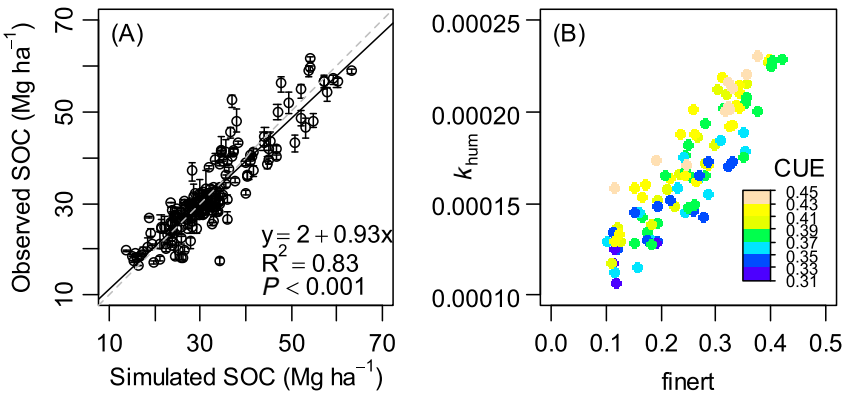

Fig. 2. Model calibration results. (A) Modelled and observed soil organic carbon in the top 30 cm soil in 90 trials at 28 sites across the Australian cropping regions. Dashed line shows the 1:1 line. Bars show the corresponding 95% confidence intervals of 100 simulations of SOC using the 100 ensembles of parameters shown in (B). (B) Calibrated model parameters. k_{hum}, the decay constant of the humic organic matter; *finert*, the fraction of inert organic matter in total soil organic matter; *CUE*, the carbon use efficiency of microbes.

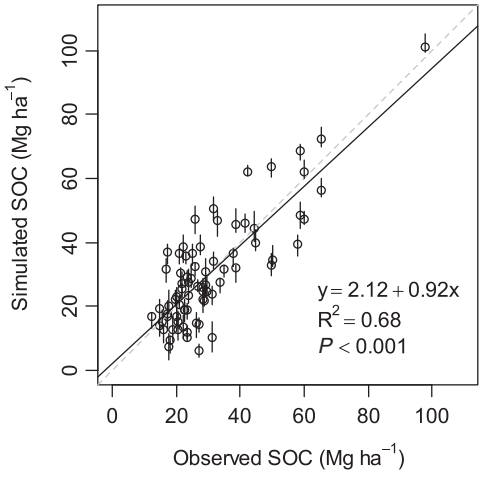

Fig. 3. Model validation results. The modelled and observed soil organic carbon in the top 30 cm soil in 75 trials at 46 sites.

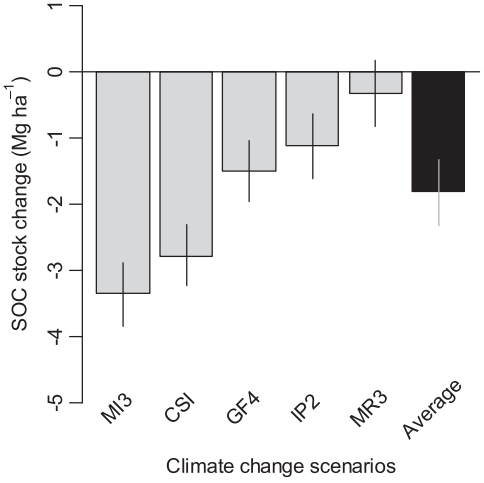

Fig. 4. National SOC changes during the period 2009–2070 in Australian rainfed croplands under five climate projections and their average. Error bars show the 95% confidence intervals. See Table S2 for the five climate projections.

collinearity leads to different combinations of model parameters generating the same result of SOC dynamics shown in Fig. 2a. When the calibrated model was applied to an independent data set, it was able to explain 68% (P < 0.001) of the variances in observed SOC stocks (Fig. 3). Using the parameter ensembles (Fig. 2B), the model also simulated crop growth well (Fig. S1).

Applying the calibrated and validated APSIM model to the 1869 randomly selected points, SOC dynamics were predicted during the period 2009–2070. The average change of SOC (i.e., Δ*SOC*) during the period was predicted to be −1.81 Mg C ha^{-1} over the 60 years, with the 95% CI ranging from −2.32 to −1.32 Mg C ha^{-1} by considering the uncertainties in model parameter estimation and climate projection (Fig. 4). The five climate projections had a significant effect on the predicted Δ*SOC*, but the difference of Δ*SOC* between the five GCMs was small and Δ*SOC* was significantly negative for all climate projections except the MR3 (Fig. 4). Although the average Δ*SOC* at the simulated points was negative (Fig. 4), the simulations across the 1869 points revealed great spatial variability in Δ*SOC* (Fig. 5A, B and C). In general, Δ*SOC* increased (from negative to positive) from southwest to northeast in Western Australia; and decreased (from positive to negative) from southeast to northwest in eastern Australia. In terms of Δ*SOC* at each point, its mean ranged from −108.8 to 9.89 Mg ha^{-1} (Fig. 5B), while its upper limit of the 95% CI ranged from −96.3 to 22.2 Mg ha^{-1} (Fig. 5A) and lower limit from −123.1 to 3.71 Mg ha^{-1} (Fig. 5C). Particularly, Δ*SOC* was always negative (i.e., a carbon source) in the most northern regions of eastern Australia, while Δ*SOC* was always positive (i.e., a carbon sink) in the northeast cropping areas of Western Australia (Fig. 5).

Assessing the relative contributions of model parameterization and climate projections to the uncertainty in Δ*SOC*, the results indicated that the uncertainty was mainly attributed to parameter equifinality (Fig. 6), particularly in Western Australia and southern regions of eastern Australia (Fig. 6A). Although the contributions varied greatly among simulated points, in 72% of the simulated points, the relative contribution of model parameterization to the uncertainty was > 50% (Fig. 6B). Averaging across the simulated points, parameter equifinality accounted for 65% of the total uncertainty.

The spatial variability of APSIM-predicted Δ*SOC* across the 1869 points was well-captured by surrogate models of the APSIM model, which was the best model selected by a repeated 10-fold cross validation (Fig. 7). The surrogate models driven by initial SOC stock (SOC_0), local historical annual average temperature and rainfall during the period 1976–2005, and five variables indicating cropping system characteristics could explain > 97% of the variance in APSIM-predicted upper limit (Fig. 7A), average (Fig. 7B), and lower limit (Fig. 7C) of Δ*SOC*. However, the magnitude (even the direction particularly for the upper limit, Fig. 7D, E and F) of the correlation coefficients (i.e., the change in Δ*SOC* per unit change in the predictor) varied greatly among the 23 AERs (i.e., 23 cropping systems, Fig. 7). The effects of the five indicators of cropping systems were consistent among the average, upper and lower limits: increasing pasture frequency and nitrogen fertilizer application rate had a positive effect on Δ*SOC*, while increasing fallow period had a negative effect (Fig. 7D, E and F). The 10-fold cross validation (which was repeated by 10 times) of the surrogate model showed negligible difference in the model performance. The root mean squared prediction error (RMSE) of the repeated cross validation

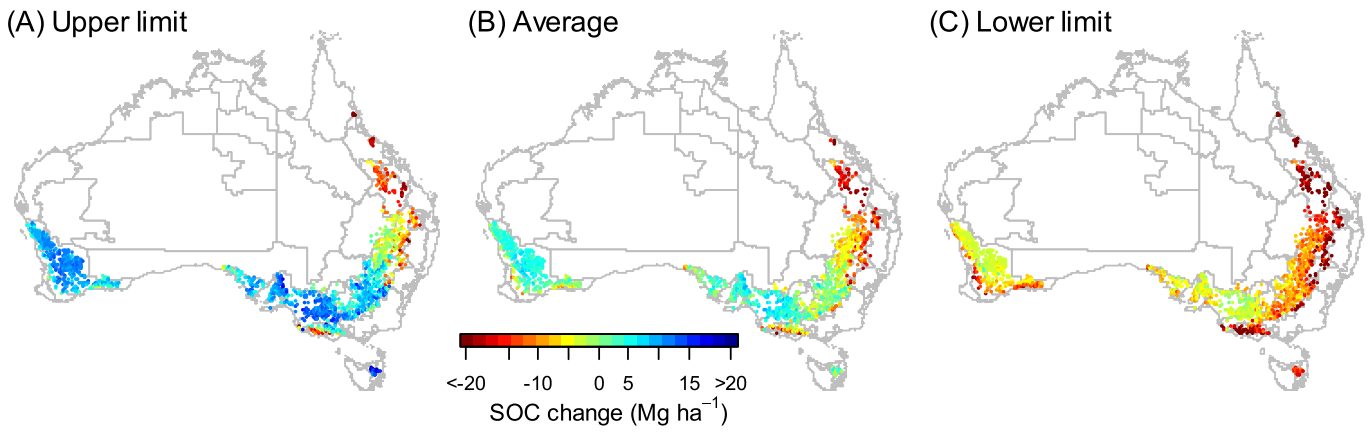

Fig. 5. The spatial pattern and uncertainty of SOC change during the period 2009–2070 at 1869 points. (A), (B) and (C) show the upper, average, and lower limits of the 95% confidence intervals. The uncertainty includes that induced by model parameterization and future climate projections.

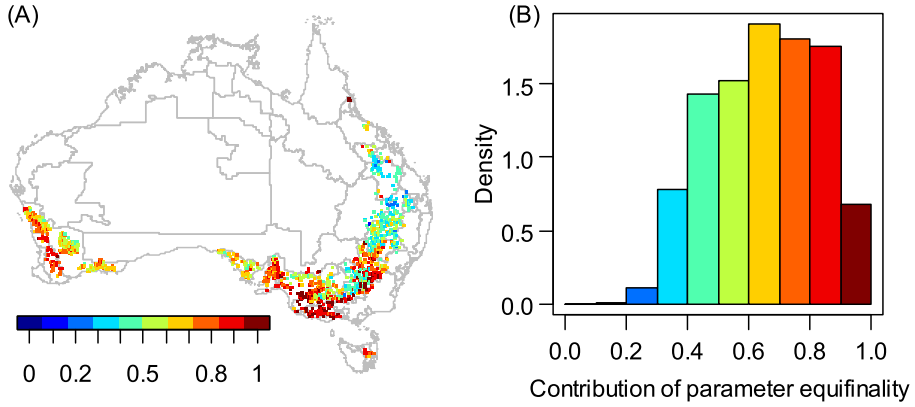

Fig. 6. The fraction of uncertainty induced by model parameter equifinality. (A) The spatial pattern. (B) The probability density distribution. A value of 0.5 indicates that 50% of the uncertainty attributes to parameter equifinality, and the left 50% attributes to climate projections.

ranged from 1.546 to 1.566 kg ha^{-1} for the upper limit (Fig. 7A), from 1.261 to 1.276 kg ha^{-1} for the average (Fig. 7B), from 1.394 to 1.404 kg ha^{-1} for the lower limit (Fig. 7D), further demonstrating the predictive power of the surrogate model.

Fig. 8 presents the results of implementing the surrogate models across the whole study region (i.e., rainfed cropping areas in Australia) at the resolution of 1 km. At the national level, average ΔSOC was -0.66 Mg ha^{-1} with the 95% CI ranging from -8.39 to 5.79 Mg ha^{-1}. For the upper limit, average and lower limit of ΔSOC across the 23 AERs, they ranged from -96.61 to 29.91 Mg ha^{-1}, -107.90 to 13.14, and -121.20 to 5.01, respectively. These ranges were generally comparable with that of the 1869 simulation points. Table S1 shows ΔSOC in each AER based on the surrogate modelling results. Among the 23 AERs, only five AERs showed average increase of SOC and the amount of the increase was relatively small (< 5 Mg ha^{-1}). In contrast, SOC in other AERs showed relatively large losses reaching to an average loss of 49.58 Mg ha^{-1} in AER No. 25 (Northern Queensland Tablelands), followed by No. 21 (Central Queensland coast) and No. 19 (Wide Bay Burnett, Queensland) where the SOC losses were > 20 Mg ha^{-1} on average during the simulated 62 years (Table S1).

4. Discussion

4.1. SOC balance in Australian croplands in the period 2009–2070

This study is the first to comprehensively predict SOC dynamics in Australian rainfed cropping regions under climate change using an approach of combining farming system modelling and surrogate modelling. We found that, at the national level, Australian rainfed cropping soils under current common agricultural practices will be a source of atmospheric CO_2 on average. However, this C source is relatively small, with national average CO_2 emissions to the atmosphere of 0.66 Mg^{-1}C ha^{-1} (i.e., a 0.00017 Pg C reduction of the 0.011 Pg SOC stock in whole Australian rainfed cropping systems). This reduction (i.e., 1.5%) is much smaller than the predictions in similar land uses in Europe. Smith et al. (2005) predicted that the cropland SOC stock in Europe may decrease from 11 Pg in 1990 to 5–7 Pg in 2080. In the North Central Region of the USA, a major region for wheat, corn and soybean production, an average reduction of ~6% was predicted during the period 1990–2100 (Grace et al., 2006). In contrast, Yu et al. (2013), using the Agro-C model, predicted that croplands in China will be a C sink in the period 2011–2050. These variable predictions across different regions suggest that the different agricultural management practices, and edaphic and climatic conditions must be considered for assessing SOC dynamics in agroecosystems.

The small change of SOC stock in Australian agricultural soils under current management practices may suggest that they have great potential for carbon sequestration, because the current management practices are not optimal. Particularly, the crop residue retention fraction was only 86% at the national level, and the national average fertilizer application rate was only 38 kg N ha^{-1} indicating that Australian agricultural production may be largely N-limited. As both residue retention rate and fertilizer amount affect C input to the soil, improving these management factors may convert Australian rainfed croplands from a net carbon source to a net carbon sink of atmospheric CO_2. Indeed, our previous studies in the same region have

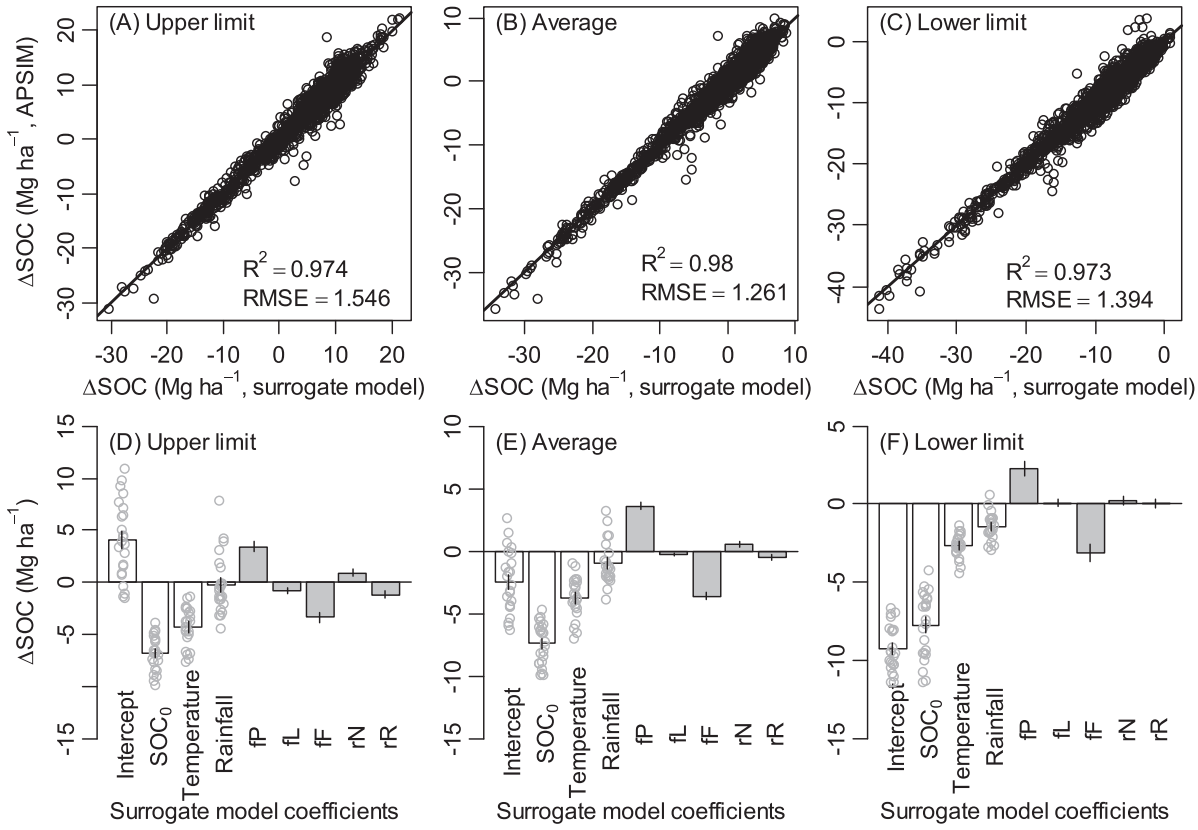

Fig. 7. The performance of surrogate models (upper panels) and their coefficients (lower panels). The surrogate models are the best model selected via 10-fold cross-validation repeated 10 times, and RMSE is the root mean squared prediction error of the surrogate model. Open bars show coefficients of initial SOC stock (SOC_0), temperature and rainfall for random effects. Grey circles show the variability of the coefficients across 23 agro-ecological regions with different cropping systems, while bars show their average with their standard deviations (the vertical error bars). The points are jittered on the x-axis by adding a small random number to avoid overlapping of the points. Grey bars show the coefficients of five predictors for fixed effects. Please refer to the text for the details of the surrogate model.

demonstrated that SOC in Australian wheat croplands can be increased by 16% on average if all residues are retained and more N fertilizer is applied to obtain the water-limited yield potential (Luo et al., 2013; Luo et al., 2017c). Assuming this increase occurs in 50 years, the yearly increase is 3.2‰, which is comparable with the 4‰ target of the "4 per 1000" initiative (Minasny et al., 2017).

4.2. Uncertainty sources in future SOC predictions

We found that the relative contributions of model parameters and climate projections vary greatly among simulated points (Fig. 6). Averaging across the points, 35% of the uncertainty was attributed to climate projections, while model parameter equifinality accounted for the remaining 65%. This result suggests that robust climate projections are required in order to reduce uncertainty in SOC predictions. As climate projections strongly rely on GCMs, it is important to select the GCMs that are capable of reproducing relevant weather patterns for the impact sector of interest. Das Bhowmik et al. (2017) proposed an approach to derive the most likely probabilistic climate projection by weighting the performance of various GCMs in long-term simulations, providing a promising solution for more reliable climate projections and thus reducing uncertainties in SOC predictions.

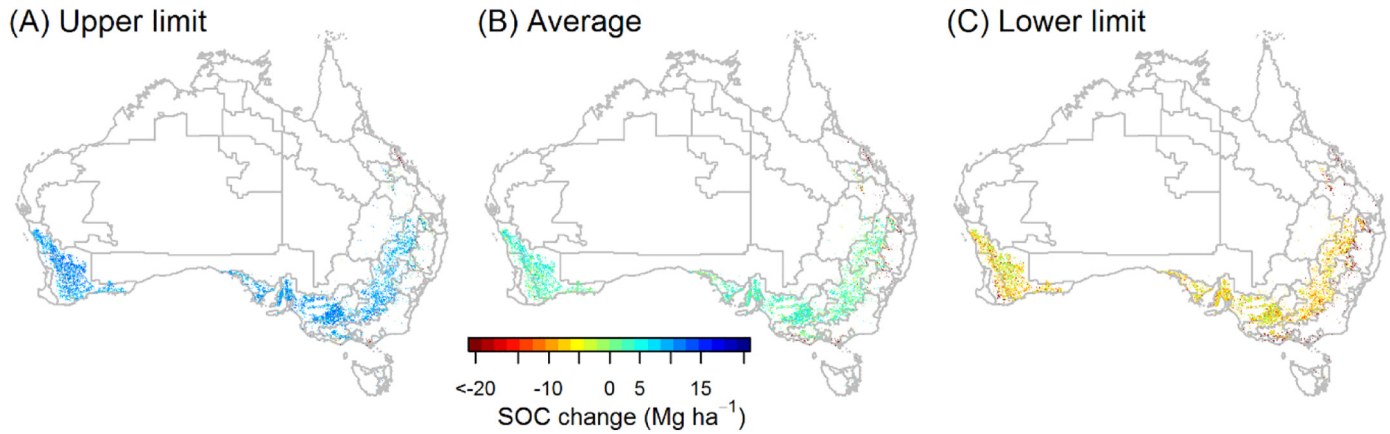

Fig. 8. SOC change during the period 2009–2070 predicted by surrogate models across the whole Australian cropping areas at each 1 km grid cell. (A), (B) and (C) show the upper, average, and lower limits of the 95% confidence intervals.

However, our results demonstrate the climate projection is much less important than parameter equifinality. To reduce uncertainty in future SOC predictions, a major task for the modelling community will be to solve the parameter equifinality issue (Luo et al., 2017b; Smith et al., 2017). Our results provide some important insights into data collection to better initialize/parameterize the model therefore reducing parameter equifinality. Observational data in line with model requirement (e.g., C pool composition and their decay rates and/or microbial C use efficiencies) are essential for improving model predictions. Once one or more parameters can be empirically determined, the collinearity issue (Fig. 2B) will be largely overcome. In the APSIM model, for example, inert organic carbon (determined by the *finert* parameter) can be replaced by measurable fractions such as charcoal C. This replacement will certainly further constrain the posterior distributions of other model parameters therefore potentially reducing uncertainty in SOC predictions. Indeed, a number of studies have demonstrated that conceptual C pools can be replaced by measurable pools (such as particulate organic matter and charcoal) (Luo et al., 2014; Zimmermann et al., 2007), which allow modelled dynamics of each pool to be directly compared with their corresponding observations other than the total SOC alone.

4.3. The power of surrogate modelling

In this study, we created parsimonious statistical emulators of the complex APSIM model, i.e., the surrogate models (Fig. 7). These surrogate models accurately reproduced the behaviour of the APSIM model in simulating SOC dynamics under different environmental conditions and agricultural management, and the prediction error of the surrogate models (which is quantified as the root mean squared error) was < 1.6, 1.3 and 1.5 kg ha^{-1} for the upper limit, average, and lower limit of the APSIM-predicted SOC change, respectively. The surrogate models are driven by a common set of easily obtainable soil and climate variables including initial SOC storage, temperature and rainfall. This correctly captured the major influencing factors on SOC dynamics in the APSIM model as initial SOC storage determines the C pool size, and temperature and rainfall determine the actual decay rate of C pools. Another set of variables reflected the effect of management practices on C input into the soil. As expected, management benefiting potential C input into the soil such as increase pasture frequency and nitrogen fertilizer application rate had a positive effect on SOC, while management limiting crop biomass production (e.g., long fallow period) or reducing crop residue retention had a negative effect on SOC (Fig. 7D, E and F). These results demonstrate the credibility of simple surrogate models to mimic the outcomes of complex process-based models.

A major application of the surrogate models is to enable the use of a cost efficient emulator of a complex process-based model across large scales at fine resolution. With fine resolution data of those easily available variables driving the surrogate models, the surrogate models can be readily applied to estimate ΔSOC in the domain that the model is developed. Using the surrogate models, the time required to generate the fine resolution regional map of SOC change and its uncertainty (Fig. 8) is shortened to several minutes, while it requires several months if running the APSIM model at each 1 km grid cell using the computing resources we had available. In addition, although we used the total SOC change during the whole 62-year simulation period to demonstrate the surrogate model development, the surrogate modelling approach can be easily expanded to reproduce time-series SOC outputs of the APSIM model and then can serve as an easy and effective tool to estimate SOC change in any typical year based on site-specific soil, climate, and agricultural management practices.

4.4. Limitations and future research

We note several limitations in our simulations, requiring additional research as well as providing insights into future studies. First, we chose only five GCMs to project the climate in the period 2009–2070 under the specific emission scenario of RCP4.5. As temperature and rainfall have a vital role in regulating SOC changes (Fig. 7) via their effects on C inputs and outputs, future SOC prediction would vary significantly depending on future emission scenarios and climate projections. For example, Wang et al. (2018) estimated the same trend of wheat (the dominant crop in Australia) production (i.e., relatively stable albeit great inter-annual variability) as our predictions under RCP4.5 (Fig. 4). Under RCP8.5, however, some studies have demonstrated that wheat production will decrease significantly in Australia (Rosenzweig et al., 2014; Wang et al., 2018). This decrease would certainly reduce C inputs to the soil therefore negatively affecting future SOC stock. The additional temperature increase under RCP8.5 compared with RCP4.5 would also stimulate C losses via microbial decomposition. For these reasons, it is reasonable to expect that more C would be lost under RCP8.5.

Second, we did not simulate the potential changes of agricultural practices and advances in agronomy. In this study, we simply repeated current crop rotations during the 62-year simulation. In reality, farmers choose crops according to price, risk of crop failure and local factors such as weeds and disease. It will be interesting to explore how the crop sequence affects SOC dynamics. In the future, conservation agricultural practices (e.g., 100% residue retention) may be more frequently adopted, thus benefiting SOC stock. Breeding efforts may also result in adaptation of crops to climate change, increased nutrient and water use efficiencies, and enhanced crop growth (Hochman et al., 2017). All these directly or indirectly affect carbon inputs to the soil and thus final SOC stock.

Last, our study does not assess all potential uncertainty sources and their relative importance and effects on the results. An especially important uncertainty source is model structure (Bradford et al., 2016; Brilli et al., 2017; Ogle et al., 2010a; Todd-Brown et al., 2013) which was not considered in this study. Most current biophysical and/or biogeochemical models including the APSIM model simulate SOC dynamics as primarily driven by temperature and moisture responses (Todd-Brown et al., 2014). The APSIM model simulates SOC dynamics using a traditional framework of first-order decay of different conceptual C pools, treating microbial and soil protection processes as black boxes. A new framework is emerging to explicitly represent microbial and physicochemical protection processes in C models (Davidson et al., 2014; Lehmann and Kleber, 2015). It will be interesting to assess the potential uncertainty induced by different model structures. This is particularly important as soil disturbance is frequent in agroecosystems, intensively influencing microbial processes and the soil environment relating to C stabilization/destabilization. How different models simulate these process may have substantial effects on predictions of SOC. Although the model performs well in general, it also should be noted that the model validation result is not as good as model calibration with a 15% reduction in model performance (68% vs 83%, Fig. 2A vs Fig. 3). When the uncertainty induced by the imperfect model performance is propagated into the surrogate models, the uncertainty in the prediction of SOC change may increase and should be properly quantified in future studies. The reduction of the model performance in simulating validation data set also suggests that extrapolating the model to the domain beyond that for which the model is calibrated may decrease the reliability of model predictions, and the model may miss some key processes controlling spatial SOC dynamics.

5. Conclusions

Using the regional-scale-constrained APSIM model and its powerful surrogates, we provided at present the most comprehensive predictions of SOC dynamics from 2009 to 2070 in Australian rainfed cropping soils under business-as-usual management practices. The soils were predicted to be a source of atmospheric CO_2 on average, but the magnitude

of this source was relatively small (0.66 Mg ha^{-1} in the period 2009–2070 on average). This value provides a benchmark for assessing soil carbon sequestration in Australian rainfed cropping systems. The ensemble simulations considering climate projections and model parameter equifinality demonstrated the importance of a reliable climate projection and further constrained parameter space for reducing uncertainties in future SOC predictions, albeit reducing parameter equifinality is more important. The derived surrogate models accurately reproduced APSIM-predicted ΔSOC and its uncertainty by correctly capturing the negative effects of temperature and rainfall on SOC decay processes and the regulation of management practices on C inputs into the soil. Applying the surrogate models across the region at the 1 km resolution, we mapped soil carbon changes under future climate conditions. This result will be particularly useful for identifying high priority regions for climate change mitigation through increasing SOC stocks and for targeting hotspots for SOC restoration.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.geoderma.2018.09.041.

References

Asseng, S., Keating, B., Fillery, I., et al., 1998. Performance of the APSIM-wheat model in Western Australia. Field Crop Res. 57, 163–179.
Baldock, J., 2012. Yield and N Estimation for Dryland Cropping. CSIRO, Canberra.
Baveye, P.C., Berthelin, J., Tessier, D., Lemaire, G., 2018. The “4 per 1000” initiative: a credibility issue for the soil science community? Geoderma 309, 118–123.
Bradford, M.A., Wieder, W.R., Bonan, G.B., Fierer, N., Raymond, P.A., Crowther, T.W., 2016. Managing uncertainty in soil carbon feedbacks to climate change. Nat. Clim. Chang. 6, 751–758.
Brilli, L., Bechini, L., Bindi, M., et al., 2017. Review and analysis of strengths and weaknesses of agro-ecosystem models for simulating C and N fluxes. Sci. Total Environ. 598, 445–470.
Das Bhowmik, R., Sharma, A., Sankarasubramanian, A., 2017. Reducing model structural uncertainty in climate model projections-a rank-based model combination approach. J. Clim. 30, 10139–10154.
Davidson, E.A., Savage, K.E., Finzi, A.C., 2014. A big-microsite framework for soil carbon modeling. Glob. Chang. Biol. 20, 3610–3620.
Freibauer, A., Rounsevell, M.D.A., Smith, P., Verhagen, J., 2004. Carbon sequestration in the agricultural soils of Europe. Geoderma 122, 1–23.
Gan, Y., Liang, C., Chai, Q., Lemke, R.L., Campbell, C.A., Zentner, R.P., 2014. Improving Farming Practices Reduces the Carbon Footprint of Spring Wheat Production. 5. pp. 5012.
Gelman, A., Hill, J., 2006. Data analysis using regression and multilevel/hierarchical models. Cambridge university press.
Grace, P.R., Colunga-Garcia, M., Gage, S.H., Robertson, G.P., Safir, G.R., 2006. The potential impact of agricultural management and climate change on soil organic carbon of the north central region of the United States. Ecosystems 9, 816–827.
Grundy, M., Rossel, R.V., Searle, R., Wilson, P., Chen, C., Gregory, L., 2015. Soil and landscape grid of Australia. Soil Res. 53, 835–844.
Guo, L.B., Gifford, R.M., 2002. Soil carbon stocks and land use change: a meta analysis. Glob. Chang. Biol. 8, 345–360.
Hochman, Z., Gobbett, D.L., Horan, H., 2017. Climate trends account for stalled wheat yields in Australia since 1990. Glob. Chang. Biol. 23, 2071–2081.
Holzworth, D.P., Huth, N.I., Zurcher, E.J., et al., 2014. APSIM–evolution towards a new generation of agricultural systems simulation. Environ. Model. Softw. 62, 327–350.
Huth, N.I., Thorburn, P.J., Radford, B.J., Thornton, C.M., 2010. Impacts of fertilisers and legumes on N_2O and CO_2 emissions from soils in subtropical agricultural systems: a simulation study. Agric. Ecosyst. Environ. 136, 351–357.
Kahiluoto, H., Smith, P., Moran, D., Olesen, J.E., 2014. Enabling food security by verifying agricultural carbon. Nat. Clim. Chang. 4, 309–311.
Kong, A.Y., Six, J., Bryant, D.C., Denison, R.F., Van Kessel, C., 2005. The relationship between carbon input, aggregation, and soil organic carbon stabilization in sustainable cropping systems. Soil Sci. Soc. Am. J. 69, 1078–1085.
Kucharik, C.J., Brye, K.R., Norman, J.M., Foley, J.A., Gower, S.T., Bundy, L.G., 2001. Measurements and modeling of carbon and nitrogen cycling in agroecosystems of southern Wisconsin: potential for SOC sequestration during the next 50 years. Ecosystems 4, 237–258.
Lal, R., 2004. Soil carbon sequestration impacts on global climate change and food security. Science 304, 1623–1627.
Lehmann, J., Kleber, M., 2015. The contentious nature of soil organic matter. Nature 528, 60–68.
Liu, D.L., Zuo, H., 2012. Statistical downscaling of daily climate variables for climate change impact assessment over New South Wales, Australia. Clim. Chang. 115, 629–666.
Liu, D.L., Chan, K.Y., Conyers, M.K., 2009. Simulation of soil organic carbon under different tillage and stubble management practices using the Rothamsted carbon model. Soil Tillage Res. 104, 65–73.
Liu, D.L., Zeleke, K.T., Wang, B., Macadam, I., Scott, F., Martin, R.J., 2017. Crop residue incorporation can mitigate negative climate change impacts on crop yield and improve water use efficiency in a semiarid environment. Eur. J. Agron. 85, 51–68.
Luo, Z., Wang, E., Sun, O.J., 2010. Soil carbon change and its responses to agricultural practices in Australian agro-ecosystems: a review and synthesis. Geoderma 155, 211–223.
Luo, Z.K., Wang, E.L., Sun, O.J., Smith, C.J., Probert, M.E., 2011. Modeling long-term soil carbon dynamics and sequestration potential in semi-arid agro-ecosystems. Agric. For. Meteorol. 151, 1529–1544.
Luo, Z., Wang, E., Bryan, B., King, D., Zhao, G., Pan, X., Bende-Michl, U., 2013. Meta-modeling soil organic carbon sequestration potential and its application at regional scale. Ecol. Appl. 23, 408–420.
Luo, Z., Wang, E., Fillery, I.R., Macdonald, L.M., Huth, N., Baldock, J., 2014. Modelling soil carbon and nitrogen dynamics using measurable and conceptual soil organic matter pools in APSIM. Agric. Ecosyst. Environ. 186, 94–104.
Luo, Z., Wang, E., Zheng, H., Baldock, J.A., Sun, O.J., Shao, Q., 2015. Convergent modelling of past soil organic carbon stocks but divergent projections. Biogeosciences 12, 4373–4383.
Luo, Z., Feng, W., Luo, Y., Baldock, J., Wang, E., 2017a. Soil organic carbon dynamics jointly controlled by climate, carbon inputs, soil properties and soil carbon fractions. Glob. Chang. Biol. 27, 1001–1009.
Luo, Z., Wang, E., Sun, O., 2017b. Uncertain future soil carbon dynamics under global change predicted by models constrained by total carbon measurements. Ecol. Appl. 27, 1001–1009.
Luo, Z., Wang, E., Xing, H., Smith, C., Wang, G., Cresswell, H., 2017c. Opportunities for enhancing yield and soil carbon sequestration while reducing N 2 O emissions in rainfed cropping systems. Agric. For. Meteorol. 232, 400–410.
Marie, G., Simioni, G., 2014. Extending the use of ecological models without sacrificing details: a generic and parsimonious meta-modelling approach. Methods Ecol. Evol. 5, 934–943.
Meinke, H., Hammer, G.L., Van Keulen, H., Rabbinge, R., Keating, B.A., 1997. Improving wheat simulation capabilities in Australia from a cropping systems perspective: water and nitrogen effects on spring wheat in a semi-arid environment. In: Developments in Crop Science. 25. pp. 99–112.
Minasny, B., Malone, B.P., Mcbratney, A.B., et al., 2017. Soil carbon 4 per mille. Geoderma 292, 59–86.
Mullen, K.M., Ardia, D., Gil, D.L., Windover, D., Cline, J., 2009. DEoptim: An R Package for Global Optimization by Differential Evolution.
Ogle, S.M., Breidt, F., Easter, M., Williams, S., Killian, K., Paustian, K., 2010a. Scale and uncertainty in modeled soil organic carbon stock changes for US croplands using a process-based model. Glob. Chang. Biol. 16, 810–822.
Ogle, S.M., Breidt, F.J., Easter, M., Williams, S., Killian, K., Paustian, K., 2010b. Scale and uncertainty in modeled soil organic carbon stock changes for US croplands using a process-based model. Glob. Chang. Biol. 16, 810–822.
O'Leary, G.J., Liu, D.L., Ma, Y., et al., 2016. Modelling soil organic carbon 1. Performance of APSIM crop and pasture modules against long-term experimental data. Geoderma 264, 227–237.
Probert, M.E., Delve, R.J., Kimani, S.K., Dimes, J.P., 2005. Modelling nitrogen mineralization from manures: representing quality aspects by varying C: N ratio of sub-pools. Soil Biol. Biochem. 37, 279–287.
Qiu, J.J., Li, C.S., Wang, L.G., Tang, H.J., Li, H., Van Ranst, E., 2009. Modeling impacts of carbon sequestration on net greenhouse gas emissions from agricultural soils in China. Glob. Biogeochem. Cycles 23.
Rosenzweig, C., Elliott, J., Deryng, D., et al., 2014. Assessing agricultural risks of climate change in the 21st century in a global gridded crop model intercomparison. Proc. Natl. Acad. Sci. 111, 3268–3273.
Saby, N.P.A., Bellamy, P.H., Morvan, X., et al., 2008. Will European soil-monitoring networks be able to detect changes in topsoil organic carbon content? Glob. Chang. Biol. 14, 2432–2442.
Sanderman, J., Hengl, T., Fiske, G.J., 2017. Soil carbon debt of 12,000 years of human land use. Proc. Natl. Acad. Sci. 114, 9575–9580.
Skjemstad, J., Spouncer, L.R., 2003. Integrated Soils Modelling for the National Carbon Accounting System: (estimating Changes in Soil Carbon Resulting From Changes in Land Use). Australian Greenhouse Office.
Smith, P., 2016. Soil carbon sequestration and biochar as negative emission technologies. Glob. Chang. Biol. 22, 1315–1324.
Smith, J.O., Smith, P., Wattenbach, M., et al., 2005. Projected changes in mineral soil carbon of European croplands and grasslands, 1990–2080. Glob. Chang. Biol. 11, 2141–2152.
Smith, P., Lutfalla, S., Riley, W.J., Torn, M.S., Schmidt, M.W.I., Soussana, J.F., 2017. The changing faces of soil organic matter research. Eur. J. Soil Sci. 69, 23–30.
Tang, J., Zhuang, Q., 2008. Equifinality in parameterization of process-based biogeochemistry models: a significant uncertainty source to the estimation of regional carbon dynamics. J. Geophys. Res. Biogeosci. 113.
Team, R.C., 2016. R: A language and environment for statistical computing.
Todd-Brown, K., Randerson, J., Post, W., Hoffman, F., Tarnocai, C., Schuur, E., Allison, S., 2013. Causes of variation in soil carbon simulations from CMIP5 earth system models and comparison with observations. Biogeosciences 10.

Todd-Brown, K., Randerson, J., Hopkins, F., et al., 2014. Changes in soil organic carbon storage predicted by earth system models during the 21st century. Biogeosciences 11, 2341–2356.
Unkovich, M., Baldock, J., Marvanek, S., 2009. Which crops should be included in a carbon accounting system for Australian agriculture? In: Crop and Pasture Science. 60. pp. 617–626.
Van Vuuren, D.P., Edmonds, J., Kainuma, M., et al., 2011. The representative concentration pathways: an overview. Clim. Chang. 109, 5.
Vandenbygaart, A.J., 2018. Comments on soil carbon 4 per mille by Minasny et al. 2017. Geoderma 309, 113–114.
Wang, E., Van Oosterom, E., Meinke, H., et al., 2003. The New APSIM-Wheat Model—Performance and Future Improvements. In: Proceedings of the 11th Australian Agronomy Conference. Australian Society of Agronomy Geelong, Victoria (pp Page).
Wang, G., Luo, Z., Han, P., Chen, H., Xu, J., 2016. Critical carbon input to maintain current soil organic carbon stocks in global wheat systems. Sci. Rep. 6.
Wang, B., Liu, D.L., O'Leary, G.J., et al., 2018. Australian wheat production expected to decrease by the late 21st century. Glob. Chang. Biol. 24, 2403–2415.
West, T.O., Post, W.M., 2002. Soil organic carbon sequestration rates by tillage and crop rotation: a global data analysis. Soil Sci. Soc. Am. J. 66, 1930–1946.
White, R.E., Davidson, B., Lam, S.K., Chen, D., 2018. A critique of the paper 'soil carbon 4 per mille' by Minasny et al. (2017). Geoderma 309, 115–117.
Williams, J., Hamblin, A.P., Hook, R.A., 2002. Methodologies for Their Derivation and Key Issues in Resource Management. CSIRO Land and Water.
Yu, Y., Huang, Y., Zhang, W., 2013. Projected changes in soil organic carbon stocks of China's croplands under different agricultural managements, 2011–2050. Agric. Ecosyst. Environ. 178, 109–120.
Zhao, G., Bryan, B.A., King, D., Luo, Z., Wang, E., Song, X., Yu, Q., 2013. Impact of agricultural management practices on soil organic carbon: simulation of Australian wheat systems. Glob. Chang. Biol. 19, 1585–1597.
Zimmermann, M., Leifeld, J., Schmidt, M.W.I., Smith, P., Fuhrer, J., 2007. Measured soil organic matter fractions can be related to pools in the RothC model. Eur. J. Soil Sci. 58, 658–667.